

# Fully spin-dependent boundary condition for isotropic quasiclassical Green's functions

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Transport in superconducting heterostructures is very successfully described with quasiclassical Green's functions augmented by microscopically derived boundary conditions. However, so far the spin-dependence is in the diffusive approach included only for limiting cases. Here, we derive the fully spin-dependent boundary condition completing the Usadel equation and the circuit theory. Both, material specific spin-degrees of freedom and spin-dependent interface effects, i.e. spin-mixing and polarization of the transmission coefficients are treated exactly. This opens the road to accurately describe a completely new class of mesoscopic circuits including materials with strong intrinsic magnetic structure. We also discuss several experimentally relevant cases like the tunnel limit, a ferromagnetic insulator with arbitrarily strong magnetization and the limit of small spin-mixing.

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A central question in quantum transport is to find boundary conditions (BC) defining the current across contacts of different materials, like e.g. superconducting heterostructures possibly including ferromagnetic materials. A straight forward approach to this is to match the wavefunctions at the interface (see e.g. [1]). A generalization of this approach containing many transport channels and all kinds of different barriers can be formulated with a scattering matrix [2]. However, due to the huge variety of effects in quantum transport it is in many cases more convenient to work with Green's functions (see e.g. [3]) instead of a wave functions. These Green's functions are described by the Gor'kov equations [4], which are not practically solvable in the presence of interfaces and disorder. In the quasiclassical limit (i.e. the Fermi energy is much larger than all relevant energy scales) [5] it is however possible to split the total Green's into a ballistic part that is continuous at the interface and can thus be described within a scattering approach and a discontinuity [6]. In this way, BCs for quasiclassical Green's functions can be formulated. A generalization to this approach for magnetically active interfaces is given in [7], leading to a pair breaking effect of a magnetic insulator due to the spin-mixing [8]. Junctions including strongly diffusive superconductors are treated in [9]. A more detailed overview can be found in [10, 11], where the need for a BC the covers superconductor-strong ferromagnet interfaces was pointed out.

As already implied, for many physical systems like superconducting heterostructures mainly two limits are considered. The clean (ballistic) limit that assumes the transport to be described by ballistic trajectories and the dirty (diffusive) limit where the mean-free path is the smallest length scale in the system and the transport inside the leads is dominated by the impurity self-energy from Born's approximation. A BC for stationary problems that covers spin-dependent effects based on a scattering approach within the clean limit is given in [12]. The aim of this paper is to provide a fully derived, general

BC within the framework of quasiclassical Green's functions in the case of strongly diffusive materials. The dirty limit BC for the spin-independent case is already known since long [13]. In this theory (called quantum circuit theory) a matrix-current in Nambu-Keldysh space [14, 15] is defined for which generalized Kirchhoff's rules apply as a direct consequence of the discretization of the Usadel equation [16]. Observable currents (like charge, energy and spin currents) are then defined from the energy integral over subtraces of the matrix-current. An extension of these BC's that consider spin-dependent effects to first order in the tunneling is provided in [17–19]. Another extension that doesn't consider spin mixing but an interface polarization is found in [20]. However, a BC that treats all the spin-dependent effects exactly is still missing. We note that further works consider time-dependent scattering [21] or spin-dependent effects in specific models [12, 24–27].

The derivations in this manuscript are mainly based on the ideas presented in [13] and [18]. Thus the results represent a generalizations of the Nazarov boundary condition for spin-dependent problems.

Throughout the paper we indicate all operators with non-trivial structure in more than one subspace by their decorations according to table I. We will use  $\sigma/\tau/\Sigma$  for the Pauli-matrices in Spin-/Nambu-/Direction (of propagation)-space respectively. We work in the Spinor-basis  $\Psi^\dagger = (\psi_\uparrow^\dagger, \psi_\downarrow^\dagger, -\psi_\downarrow, \psi_\uparrow)$ . Thus, we defined the time-reversal operator as  $R = -i\sigma_2 R_0$ , where for any  $\bar{A}$  the operator  $R_0$  yields the complex conjugate ( $R_0 \bar{A} = \bar{A}^*$ ).

In this basis the transfer matrix  $\tilde{\mathcal{M}}$  that transfers states  $(\varphi^{L/R})^T = ((\varphi^{L/R})^e, (\varphi^{L/R})^h)$  ( $L/R$  label the left/right side of the interface,  $e/h$  labels the electron/hole component) like  $\varphi^R = \tilde{\mathcal{M}}\varphi^L$  has the following structure in Nambu space:

$$\tilde{\mathcal{M}} = \begin{pmatrix} \bar{\mathcal{M}}^e & 0 \\ 0 & \bar{\mathcal{M}}^h \end{pmatrix} = \begin{pmatrix} \bar{\mathcal{M}}^e & 0 \\ 0 & -i\sigma_2 (\bar{\mathcal{M}}^e)^* i\sigma_2 \end{pmatrix}. \quad (1)$$

The transfer matrix is equivalent to the scattering ma-

trix and can be found using the unitarity condition. As shown in [18], the transfer matrix  $\tilde{M}$  relating the ballistic Green's functions like  $\hat{g}^R = \tilde{M}\hat{g}^L\tilde{M}^\dagger$  is defined as

$$\tilde{M} = \begin{pmatrix} \bar{\mathcal{M}}^e & 0 \\ 0 & \Sigma_1 \bar{\mathcal{M}}^h \Sigma_1 \end{pmatrix}. \quad (2)$$

Thus assuming the decomposition  $\bar{\mathcal{M}}^e = (\mathcal{M}^e)' + (\mathcal{M}^e)'' \vec{m} \vec{\sigma}$  for the electronic transfer matrix, with the magnetization unit vector  $\vec{m}$ , we find the compact form

$$\tilde{M} = \tilde{M}' + \tilde{M}'' \tilde{\kappa}. \quad (3)$$

Here we defined  $\tilde{M}' = (\mathcal{M}^e)'$ ,  $\tilde{M}'' = (\mathcal{M}^e)''$  and  $\tilde{\kappa} = \tau_3 \otimes \vec{m} \vec{\sigma}$ . To find the matrices  $\tilde{M}'$  and  $\tilde{M}''$ , we start with the most general form of the electronic transfer matrix (see e.g. [18]):

$$\bar{\mathcal{M}}_n^e = \begin{pmatrix} \frac{i}{\sqrt{\hat{T}_n}} e^{i\varphi_n/2} & -i\sqrt{\frac{1-\hat{T}_n}{\hat{T}_n}} e^{i\chi_n/2} \\ i\sqrt{\frac{1-\hat{T}_n}{\hat{T}_n}} e^{-i\chi_n/2} & \frac{-i}{\sqrt{\hat{T}_n}} e^{-i\varphi_n/2} \end{pmatrix} \quad (4)$$

The index  $n$  labels the transport channel. We assumed the transfer matrix to be already diagonalized in channel space[22], which is always possible since the isotropic Greens functions are structureless in that space. Note that the transfer matrix includes channel-dependent polarizations of the transmission coefficients  $P_n$ , spin-dependent phase shifts (spin mixing angles)  $\delta\phi_n^{L/R}$  and even the spin-quantization axes  $\vec{m}_n$ . Explicitly we defined  $\hat{T}_n = T_n(1 + P_n \vec{m}_n \vec{\sigma})$  and  $\dot{\phi}_n^{L/R} = \phi_n^{L/R} + (\delta\phi_n^{L/R}/2) \vec{m}_n \vec{\sigma}$ , while  $\dot{\varphi}_n = \dot{\phi}_n^R + \dot{\phi}_n^L$  and  $\dot{\chi}_n = \dot{\phi}_n^R - \dot{\phi}_n^L$ .

The desired form of  $\bar{\mathcal{M}}^e$ , Eq. (3) is found using the matrix structure of  $\vec{m} \vec{\sigma}$  to rewrite the prefactor of the matrix elements in Eq. (4) according to

$$\frac{1}{\sqrt{\hat{T}}} = \frac{1}{\sqrt{T'}} (p_+ - p_- \vec{m} \vec{\sigma}) \quad (5)$$

$$\sqrt{\frac{1-\hat{T}}{\hat{T}}} = \frac{1}{\sqrt{T'}} (t_+ - t_- \vec{m} \vec{\sigma}) \quad (6)$$

with

$$T' = T(1 - P^2) \quad (7)$$

$$p_{+/-} = \text{sign} P^{0/1} \sqrt{\frac{1}{2}(1 \pm \sqrt{1 - P^2})} \quad (8)$$

$$t_{+/-} = \text{sign} P^{0/1} \sqrt{\frac{1}{2}(1 - T' \pm \sqrt{(1 - T')^2 - P^2})}. \quad (9)$$

Note that all these quantities (transmission, magnetization, polarization, phases and phase shifts) are diagonal but non-trivial matrices in the channel subspace. We expand Eq. (3) with the help of Eqs. (4), (5), and (6) and

	$\hat{A}$	$\hat{A}$	$\hat{A}$	$\hat{A}$	$\hat{A}$	$\hat{A}$	$\hat{A}$	$\hat{A}$
spin	✓	✗	✓	✓	✓	✓	✓	✓
Nambu	✗	✗	✓	✓	✓	✗	✓	✓
direction	✗	✓	✗	✗	✗	✓	✓	✓
Keldysh	✗	✗	✓	✗	✓	✗	✗	✓
channel	✓	✓	✗	✓	✓	✓	✓	✓

TABLE I: Explanation of decorations used throughout the paper. The symbols ✓ and ✗ indicate that the operator has or has no structure in the particular subspace.

find

$$M'_{11} = (\tilde{M}')_{11} = \frac{i}{\sqrt{T'}} e^{i\varphi/2} (p_+ c_\varphi - i p_- s_\varphi) \quad (10)$$

$$M''_{11} = (\tilde{M}'')_{11} = \frac{i}{\sqrt{T'}} e^{i\varphi/2} (-p_- c_\varphi + i p_+ s_\varphi) \quad (11)$$

$$M'_{12} = (\tilde{M}')_{12} = \frac{-i}{\sqrt{T'}} e^{i\chi/2} (t_+ c_\chi - i t_- s_\chi) \quad (12)$$

$$M''_{12} = (\tilde{M}'')_{12} = \frac{-i}{\sqrt{T'}} e^{i\chi/2} (-t_- c_\chi + i t_+ s_\chi). \quad (13)$$

We defined  $c_\alpha = \cos(\delta\alpha/4)$  and  $s_\alpha = \sin(\delta\alpha/4)$ . All other components are related by further symmetries (equivalent to the unitarity of the scattering matrix):

$$M'_{22} = (M'_{11})^* ; M''_{22} = (M''_{11})^* \\ M'_{21} = (M'_{12})^* ; M''_{21} = (M''_{12})^*.$$

The matrix-current in the isotropization zone on the left/right side of the contact is found in [13, 18]. For simplicity we define  $\hat{G} = \hat{G}^{L/R}$ ,  $\hat{G}' = \hat{G}^{R/L}$ , and  $\bar{K} = \bar{K}^{L/R}$ , where the indices  $L/R$  label the left/right side of the interface respectively and  $\hat{G}^{L/R}$  are the quasiclassical Green's functions of either sides. With these definitions and defining the conductance quantum  $G_Q = e^2/h$ , the matrix-current ( $\hat{I} = \hat{I}^{L/R}$ ) is

$$\hat{I} = 4G_Q \text{Tr}_{n,s} [(1 + \hat{G}\bar{K})^{-1} (\hat{G}\Sigma_3 \pm 1) \mp \frac{1}{2}], \quad (14)$$

with

$$\bar{K} = (\tilde{M}^\dagger)^{\pm 1} \hat{G}' \tilde{M}^{\pm 1}. \quad (15)$$

The index  $s$  labels the trace in direction subspace. For later usage we mention that due to  $\tilde{M}^\dagger \Sigma_3 \tilde{M} = \tilde{M} \Sigma_3 \tilde{M}^\dagger = \Sigma_3$  and the normalization condition  $(\hat{G})^2 = 1$ , it is:

$$(\Sigma_3 \bar{K})^2 = 1. \quad (16)$$

The inverse of the 2x2 matrix in the direction subspace in Eq. (14) is found in terms of components  $\check{K}_{ij}$  of  $\bar{K}$  as follows. We define

$$\bar{D}^{-1} = (1 + \hat{G}\bar{K})^{-1} \\ = \begin{pmatrix} 1 + \hat{G}\check{K}_{11} & \hat{G}\check{K}_{12} \\ \hat{G}\check{K}_{21} & 1 + \hat{G}\check{K}_{22} \end{pmatrix}^{-1} = \begin{pmatrix} (\check{D}^{-1})_{11} & (\check{D}^{-1})_{12} \\ (\check{D}^{-1})_{21} & (\check{D}^{-1})_{22} \end{pmatrix}. \quad (17)$$

Performing the trace over the  $s$ -subspace in Eq. (14) we find:

$$\hat{I} = 4G_Q \text{Tr}_n[(\check{D}^{-1})_{11}(\hat{G} \pm 1) - (\check{D}^{-1})_{22}(\hat{G} \mp 1) \mp 1]. \quad (18)$$

The entries of the 2x2 matrix  $\bar{D}^{-1}$  are found by direct inversion:

$$(\check{D}^{-1})_{11} = (1 + \hat{G}\check{K}_{11} - \hat{G}\check{K}_{12}(1 + \hat{G}\check{K}_{22})^{-1}\hat{G}\check{K}_{21})^{-1} \quad (19)$$

$$(\check{D}^{-1})_{22} = (1 + \hat{G}\check{K}_{22} - \hat{G}\check{K}_{21}(1 + \hat{G}\check{K}_{11})^{-1}\hat{G}\check{K}_{12})^{-1}. \quad (20)$$

Using the matrix structure of  $\bar{K}$  (Eq. (16)), i.e.  $\check{K}_{21}^{-1}\check{K}_{22} = \check{K}_{11}\check{K}_{21}^{-1}$  and  $\check{K}_{21}^{-1} + \check{K}_{12} = \check{K}_{11}\check{K}_{21}^{-1}\check{K}_{22}$ , Eqs. (19) and (20) can be decomposed according to:

$$(\check{D}^{-1})_{11} = \check{C}\check{A}^{-1} \quad (21)$$

$$(\check{D}^{-1})_{22} = \check{A}^{-1}(\check{K}_{21}^{-1}\hat{G} + \hat{G}\check{K}_{11}\check{K}_{21}^{-1}\hat{G}) \quad (22)$$

with

$$\check{C} = (\hat{G}\check{K}_{21})^{-1}(1 + \hat{G}\check{K}_{22}) = \check{K}_{21}^{-1}\hat{G} + \check{K}_{11}\check{K}_{21}^{-1} \quad (23)$$

$$\begin{aligned} \check{A} &= \check{K}_{21}^{-1}\hat{G} + \hat{G}\check{K}_{11}\check{K}_{21}^{-1}\hat{G} + \check{K}_{21}^{-1}\check{K}_{22} \\ &\quad + \hat{G}\check{K}_{11}\check{K}_{21}^{-1}\check{K}_{22} - \hat{G}\check{K}_{12})^{-1} \\ &= \check{C} + \hat{G}\check{C}\hat{G}. \end{aligned} \quad (24)$$

Plugging Eqs. (21), (22), (23), and (24) into Eq. (18), replacing the last summand  $\mp 1$  in Eq. (18) by  $A^{-1}A$  and

using the relation  $[A^{-1}, \hat{G}] = 0$  it is straight forward to show that [28]

$$\begin{aligned} \hat{I} &= 4G_Q \text{Tr}_n[(1 \pm \check{K}_{11})(\check{K}_{21})^{-1}, \\ &\quad \{(\hat{G} + \check{K}_{11})(\check{K}_{21})^{-1}, \hat{G}\}^{-1}(\hat{G} \pm 1)]. \end{aligned} \quad (25)$$

This is the most general form of the desired boundary condition, and thus the main result of the paper. To solve physical problems, we still need to find the components of  $\bar{K}$  to be plugged into Eq. (25). For this we plug Eq. (3) into Eq. (15) (note that  $\det \tilde{M} = 1$ ):

$$\begin{aligned} \bar{K} &= ((\hat{M}')^\dagger)^{\pm 1}(\hat{M}')^{\pm 1}\hat{G}' + ((\hat{M}'')^\dagger)^{\pm 1}(\hat{M}'')^{\pm 1}\check{\kappa}\hat{G}'\check{\kappa} \\ &\quad + ((\hat{M}')^\dagger)^{\pm 1}(\hat{M}'')^{\pm 1}\hat{G}'\check{\kappa} + ((\hat{M}'')^\dagger)^{\pm 1}(\hat{M}')^{\pm 1}\check{\kappa}\hat{G}'. \end{aligned} \quad (26)$$

The last two summands are related by the symmetry  $((\hat{M}')^\dagger)^{\pm 1}(\hat{M}'')^{\pm 1})^\dagger = ((\hat{M}'')^\dagger)^{\pm 1}(\hat{M}')^{\pm 1}$ . Plugging Eqs. (10), (11), (12) and (13) into Eq. 26 using all the symmetries one finds the following for the desired components of  $\bar{K}$ :

$$\check{K}_{11} = K'_{11}\hat{G}' + K''_{11}\check{\kappa}\hat{G}'\check{\kappa} + K'''_{11}\hat{G}'\check{\kappa} + K''''_{11}\check{\kappa}\hat{G}' \quad (27)$$

$$\check{K}_{21} = K'_{21}\hat{G}' + K''_{21}\check{\kappa}\hat{G}'\check{\kappa} + K'''_{21}\{\hat{G}', \check{\kappa}\} \quad (28)$$

with

$$(K'_{11})^L = -\frac{1}{2} + \frac{1}{T'} \left[ 1 \pm \frac{1}{2} \left\{ \sqrt{1 - P^2} \cos(\delta\varphi/2) + \sqrt{(1 - T')^2 - P^2} \cos(\delta\chi/2) \right\} \right] \quad (29)$$

$$(K''_{11})^L = \frac{1}{T'} \left[ -P + \frac{i}{2} \left\{ \sqrt{1 - P^2} \sin(\delta\varphi/2) - \sqrt{(1 - T')^2 - P^2} \sin(\delta\chi/2) \right\} \right] \quad (30)$$

$$\begin{aligned} (K'_{21})^L &= -\frac{1}{T'} e^{i\phi^L} [(p_+t_+ + p_-t_-) \cos(\delta\phi^L/2) \pm (p_+t_+ - p_-t_-) \cos(\delta\phi^R/2) \\ &\quad - i \{ (p_-t_+ + p_+t_-) \sin(\delta\phi^L/2) \mp (p_+t_- - p_-t_+) \sin(\delta\phi^R/2) \}] \end{aligned} \quad (31)$$

$$(K''_{21})^L = \frac{1}{T'} e^{i\phi^L} [(p_+t_- + p_-t_+) \cos(\delta\phi^L/2) - i(p_+t_+ + p_-t_-) \sin(\delta\phi^L/2)] \quad (32)$$

Here we partly used Eqs. (8) and (9). Due to the structure of the transfer-matrix the right-side coefficients are given by  $(K'_{ab})^R = R_0(K'_{ab})^L|_{L \leftrightarrow R}$ . Now we can express the full boundary condition with  $(\phi = \phi^{L/R}, \phi' = \phi^{R/L}, \delta\phi = \delta\phi^{L/R}, \delta\phi' = \delta\phi^{R/L})$

$$\begin{aligned} \check{K}_{11} &= (\hat{G}' + \check{\kappa}\hat{G}'\check{\kappa}) \left[ \frac{1 - P\check{\kappa}}{T'} - \frac{1}{2} \right] \\ &\quad + \frac{1}{2T'} (\hat{G}' - \check{\kappa}\hat{G}'\check{\kappa}) \left[ \sqrt{1 - P^2} e^{\pm i\check{\kappa}(\delta\phi + \delta\phi')/2} + \sqrt{(1 - T')^2 - P^2} e^{\pm i\check{\kappa}(\delta\phi - \delta\phi')/2} \right] \end{aligned} \quad (33)$$

$$\begin{aligned} \check{K}_{21} &= -\frac{1}{T'} e^{\pm i\phi} \left\{ (\hat{G}' + \check{\kappa}\hat{G}'\check{\kappa}) [p_+t_+ + p_-t_- - \check{\kappa}(p_+t_- + p_-t_+)] e^{\pm i\check{\kappa}\delta\phi/2} \right. \\ &\quad \left. + (\hat{G}' - \check{\kappa}\hat{G}'\check{\kappa}) [(p_+t_+ - p_-t_-) \cos(\delta\phi'/2) \pm i(p_+t_- - p_-t_+) \sin(\delta\phi'/2)] \right\}. \end{aligned} \quad (34)$$

This completes the central result of our work. Plugging

Eqs. (33) and (34) into Eq. (25) yields the dirty limit

matrix current through a contact where both sides ( $\hat{G}^R$  and  $\hat{G}^L$ ) can have a non-trivial structure in Nambu and spin space and the spin-dependent interface effects i. e. spin mixing and spin filtering are treated exactly. It completes the discrete version of the Usadel equation [13] to yield a complete scheme to describe a large variety of superconductor-ferromagnet heterostructures, with external fields under equilibrium and non-equilibrium conditions.

In the remainder of the paper we discuss several practically relevant simplifications of the general boundary conditions. At first we note that the Nazarov boundary condition [13] is reproduced for  $\delta\phi = \delta\phi' = P = 0$ , where  $\check{K}_{11} = (2 - T)\hat{G}'/T$  and  $\check{K}_{21} = -2\sqrt{1 - T}\hat{G}'/T$ . Thus,

with  $[\hat{G}', (\frac{T}{2(T-2)}\{\hat{G}', \hat{G}\} - 1)^{-1}] = 0$ , Eq. (25) reduces to the well-known result

$$\hat{I} = 4G_Q \sum_n \frac{T_n[\hat{G}', \hat{G}]}{4 + T_n(\{\hat{G}', \hat{G}\} - 2)}. \quad (35)$$

In many cases tunnel barriers (with or without a magnetic structure) are an experimentally realized and we will at first take the tunnel limit ( $T_n \ll 1$ ) by linear expansion of Eqs. (33) and (34):

$$T'\check{K}_{11/21} \approx \check{K}_{11/21}^0 + \check{K}_{11/21}^1 T \quad (36)$$

with

$$\check{K}_{11}^0 = (1 - P\check{\kappa})(\hat{G}' + \check{\kappa}\hat{G}'\check{\kappa}) + (\hat{G}' - \check{\kappa}\hat{G}'\check{\kappa})\sqrt{1 - P^2} \cos(\delta\phi'/2) e^{\pm i\check{\kappa}\delta\phi/2} \quad (37)$$

$$\check{K}_{11}^1 = -\frac{1}{2} \left[ (1 - P^2)(\hat{G}' + \check{\kappa}\hat{G}'\check{\kappa}) + \sqrt{1 - P^2}(\hat{G}' - \check{\kappa}\hat{G}'\check{\kappa}) e^{\pm i\check{\kappa}(\delta\phi - \delta\phi')/2} \right] \quad (38)$$

$$\check{K}_{21}^0 = -e^{\pm i\phi} \left[ (1 - P\check{\kappa})(\hat{G}' + \check{\kappa}\hat{G}'\check{\kappa}) e^{\pm i\check{\kappa}\delta\phi/2} + \sqrt{1 - P^2}(\hat{G}' - \check{\kappa}\hat{G}'\check{\kappa}) \cos(\delta\phi'/2) \right] \quad (39)$$

$$\check{K}_{21}^1 = \frac{e^{\pm i\phi}}{2} \left[ (1 - P^2)(\hat{G}' + \check{\kappa}\hat{G}'\check{\kappa}) e^{\pm i\check{\kappa}\delta\phi/2} + \sqrt{1 - P^2}(\hat{G}' - \check{\kappa}\hat{G}'\check{\kappa})(\cos(\delta\phi'/2) \mp iP \sin(\delta\phi'/2)) \right]. \quad (40)$$

Plugging Eq. (36) into Eq. (25) results in

$$\begin{aligned} \hat{I} = 4G_Q \text{Tr}_n [ & \check{K}_{11}^0 (\check{K}_{21}^0)^{-1}, \{ \check{K}_{11}^0 (\check{K}_{21}^0)^{-1}, \hat{G} \}^{-1} (1 - \{ (\hat{G}(1 - P^2) + \check{K}_{11}^1 - \check{K}_{11}^0 (\check{K}_{21}^0)^{-1} \check{K}_{21}^1) (\check{K}_{21}^0)^{-1}, \hat{G} \} \times \\ & \times \{ \check{K}_{11}^0 (\check{K}_{21}^0)^{-1}, \hat{G} \}^{-1} T) (1 \pm \hat{G})] + [(\pm(1 - P^2) + \check{K}_{11}^1 - \check{K}_{11}^0 (\check{K}_{21}^0)^{-1} \check{K}_{21}^1) (\check{K}_{21}^0)^{-1}, \\ & \{ \check{K}_{11}^0 (\check{K}_{21}^0)^{-1}, \hat{G} \}^{-1} (1 \pm \hat{G})] T]. \end{aligned} \quad (41)$$

Using the relation  $\forall \alpha \in \mathbb{C} : e^{-i\check{\kappa}\alpha}[\hat{G}', \check{\kappa}] = [\hat{G}', \check{\kappa}]e^{i\check{\kappa}\alpha}$  one finds

$$\check{K}_{11}^0 (\check{K}_{21}^0)^{-1} = -e^{\mp i(\phi + \check{\kappa}\delta\phi/2)} \quad (42)$$

$$\begin{aligned} \check{K}_{11}^1 + e^{\mp i\check{\kappa}\delta\phi/2} \check{K}_{21}^1 = \\ = \frac{\pm i}{2} \sqrt{1 - P^2} [\hat{G}', \check{\kappa}] (1 - P\check{\kappa}) \sin(\delta\phi'/2) = \pm \check{K}^1, \end{aligned} \quad (43)$$

and thus

$$\begin{aligned} \hat{I} = 4G_Q \sum_n [ & e^{\mp i\check{\kappa}_n \delta\phi_n/2}, \{ e^{\mp i\check{\kappa}_n \delta\phi_n/2}, \hat{G} \}^{-1} (\hat{G} \pm 1)] \\ & + T_n [ (e^{\mp i\check{\kappa}_n \delta\phi_n/2}, \{ e^{\mp i\check{\kappa}_n \delta\phi_n/2}, \hat{G} \}^{-1} \{ (\hat{G}(1 - P_n^2) \pm \check{K}_n^1) \\ & \times (\check{K}_{21}^0)_n^{-1}, \hat{G} \} \{ e^{\mp i\check{\kappa}_n \delta\phi_n/2}, \hat{G} \}^{-1} (\hat{G} \pm 1) ] \\ & - [(1 - P_n^2 + \check{K}_n^1) (\check{K}_{21}^0)_n^{-1}, \{ e^{\mp i\check{\kappa}_n \delta\phi_n/2}, \hat{G} \}^{-1} (\hat{G} \pm 1)] ]. \end{aligned} \quad (44)$$

Eq. (44) together with Eqs. (43) and (39) represents the tunnel limit of the full boundary condition (eq. (25)). In the case of a ferromagnetic insulator  $T_n \equiv 0$  only the first line in the Eq. (44) remains. Further simplifications

are found assuming small spin-mixing. We note that

$$\begin{aligned} & \left( \{ \hat{G}', \check{\kappa} \} (\check{\kappa} - P) + [\hat{G}', \check{\kappa}] \check{\kappa} \sqrt{1 - P^2} \right)^{-1} = \\ & = \frac{\{ \hat{G}', \check{\kappa} \} (\check{\kappa} + P) + [\hat{G}', \check{\kappa}] \check{\kappa} \sqrt{1 - P^2}}{4(1 - P^2)}. \end{aligned} \quad (45)$$

By expansion of Eq. (44) to first order in the spin-dependent phase shifts ( $\delta\phi_n, \delta\phi'_n$ ), using Eq. (45) we find:

$$\begin{aligned} 2\hat{I} = G_Q \sum_n [ & \pm T_n \left( (1 + \sqrt{1 - P_n^2}) \hat{G}' + P_n \{ \hat{G}', \check{\kappa}_n \} \right. \\ & \left. + (1 - \sqrt{1 - P_n^2}) \check{\kappa}_n \hat{G}' \check{\kappa}_n \right) - 2i \delta\phi_n, \hat{G} ]. \end{aligned} \quad (46)$$

This is the boundary condition as it is used in [19, 29] to calculate thermoelectric effects in ferromagnet-superconductor heterostructures.

In conclusion we have found a new boundary condition for isotropic quasiclassical Greens functions that generalizes the Nazarov boundary condition in the quantum circuit theory to spin-dependent problems. It is

presented in Eq. (25) supplemented by Eqs. (33) and (34). The new boundary condition captures e.g. non-collinear ferromagnets and triplet superconductors as terminals and fully accounts for arbitrary transmissions, polarizations and spin-mixing effects of the scattering region. In the tunnel limit the boundary condition can be simplified to Eq. (44), still fully accounting for arbitrary spin-mixing. This case also comprises ferromagnetic insulators by setting  $T_n = 0$  given by the first line of Eq. (44). The next drastic yet non-trivial simplification of the boundary condition is to linearize in the spin-dependent phase shifts given in Eq. (46). In this case the boundary condition takes a form of a commutator (similar to [17] and in [13]) and the transport coefficients just enter in averaged interface parameters  $T_n$ ,  $P_n$  and  $\delta\phi_n^{L/R}$ . Our results pave the way to investigate spin-dependent charge and heat transport and spin transport in superconducting heterostructures as well as unconventional correlations like odd-frequency triplet pairing using the most general boundary condition based on a fully microscopic derivation. Another application is to verify the details of microscopic models describing the intrinsic magnetic structure and magnetization behavior of e.g. ferromagnetic insulators.

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- [1] G. Blonder, M. Tinkham, T. Klapwijk, Phys. Rev. B, Phys. Rev. B **25**, 4515 (1982).
  - [2] C. J. Lambert, J. Phys. Cond. Mat. **3**, 6579 (1991); Y. Takane and H. Ebisawa, J. Phys. Soc. Jpn. **61**, 3466 (1992); C. W. J. Beenakker, Phys. Rev. B **46**, 12841 (1992).
  - [3] Rammer J and Smith H, Rev. Mod. Phys. **58**, 323359, (1986).
  - [4] L. P. Gor'kov, Sov. Phys. JETP **34**, 505 (1958).
  - [5] G. Eilenberger, Z. Physik **214**, 195 (1968); A. I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP **28**, 1200 (1969).
  - [6] A.V. Zaitsev, Sov. Phys. JETP **59**, 1163 (1984).

- [7] A. Millis, D. Rainer, and J. A. Sauls, Phys. Rev. B **38**, 4504 (1988).
- [8] T. Tokuyasu, J. A. Sauls, and D. Rainer, Phys. Rev. B **38**, 8823 (1988).
- [9] M. Yu. Kuprianov and V. F. Lukichev, Zh. Eksp. Teor. Fiz. **94**, 139 (1988).
- [10] A. I. Buzdin, Rev. Mod. Phys. **77**, 935 (2005).
- [11] F. S. Bergeret, A. F. Volkov, and K. B. Efetov, Rev. Mod. Phys. **77**, 1321 (2005).
- [12] M. Eschrig, J. Kopu, A. Konstandin, J.C. Cuevas, M. Fogelström, and G. Schön, Adv. Solid State Phys. **44**, 533 (2004).
- [13] Yu. V. Nazarov, Superlattices and Microstructures **25**, 1221 (1999).
- [14] Y. Nambu, Phys. Rev. **98**, 803 (1955).
- [15] L. V. Keldysh, Sov. Phys. JETP **20**, 1018 (1965).
- [16] K. D. Usadel, Phys. Rev. Lett. **25**, 507 (1970).
- [17] D. Huertas-Hernando, Yu. V. Nazarov, and W. Belzig, Phys. Rev. Lett. **88**, 047003 (2002).
- [18] A. Cottet, D. Huertas-Hernando, W. Belzig, and Yu. V. Nazarov, Phys. Rev. B **80**, 184511 (2009) ; Phys. Rev. B **83**, 139901(E) (2011).
- [19] P. Machon, M. Eschrig and W. Belzig, Phys. Rev. Lett. **110**, 047002 (2013).
- [20] F. S. Bergeret, A. Verso, and A. F. Volkov, Phys. Rev. B **86**, 214516 (2012).
- [21] I. Snyman and Yu. V. Nazarov, Phys. Rev. B **77**, 165118 (2008).
- [22] C. W. J. Beenakker, Rev. Mod. Phys. **69**, 731 (1997).
- [23] M. Eschrig, Phys. Rev. B **80**, 134511 (2009).
- [24] M. Fogelström, Phys. Rev. B **62**, 11812 (2000).
- [25] J. C. Cuevas and M. Fogelström, Phys. Rev. B **64**, 104502 (2001).
- [26] J. Kopu, M. Eschrig, J. C. Cuevas, and M. Fogelström, Phys. Rev. B **69**, 094501 (2004).
- [27] M. Eschrig and T. Löfwander, Nature Physics **4**, 138 (2008).
- [28]
$$\begin{aligned} \hat{I} &= 4G_Q \text{Tr}_n([\check{K}_{21}^{-1}, \check{A}^{-1}] \pm [\check{K}_{11}\check{K}_{21}^{-1}, \check{A}^{-1}] \\ &\quad \pm [\check{K}_{21}^{-1}, \check{A}^{-1}\hat{G}] + [\check{K}_{11}\check{K}_{21}^{-1}, \check{A}^{-1}\hat{G}]) \\ &= 4G_Q \text{Tr}_n[(1 \pm \check{K}_{11})\check{K}_{21}^{-1}, \{\check{C}, \hat{G}\}^{-1}(\hat{G} \pm 1)] \\ &= 4G_Q \text{Tr}_n[(1 \pm \check{K}_{11})\check{K}_{21}^{-1}, \\ &\quad \{(\hat{G} + \check{K}_{11})\check{K}_{21}^{-1}, \hat{G}\}^{-1}(\hat{G} \pm 1)] \end{aligned}$$
- [29] P. Machon, M. Eschrig and W. Belzig, New J. Phys. **16**, 073002 (2014).